1,1,1,3,3,3-Hexafluoro-2-propanol

920-66-1 | DTXSID1022134

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.03e-14 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.07e-01

Confidence level: 7.16e-01

Nearest Neighbors from the Training Set

Image not found
1,1,1,3,3,3-Hexafluoro-2-propanol
Measured: 2.58e-14
Predicted: 2.03e-14

Image not found
2-(Difluoromethoxy)-1,1,1,3,3,3-hexafluoropropane
Measured: 7.50e-14
Predicted: 3.74e-14

Image not found
Enflurane
Measured: 1.19e-14
Predicted: 1.24e-14

Image not found
Isoflurane
Measured: 1.51e-14
Predicted: 2.12e-14